TRANSPORT COEFFICIENTS IN NON-EQUILIBRIUM ARGON-HYDROGEN THERMAL PLASMAS

V. Rat [1], J. Aubreton [1], P. André [2], M.F. Elchinger [1], P. Fauchais [1], and A. Lefort [2]

[1] *SPCTS University of Limoges, 123 av. A. Thomas, 87060 Limoges cedex, France*
[2] *LAEPT Blaise Pascal University, 24 av. des Landais, 63177 Aubière cedex, France*

ABSTRACT

Transport coefficients in non-equilibrium argon-hydrogen thermal plasmas, where the kinetic temperature of electrons T_e is different from that of heavy species T_h, are calculated at atmospheric pressure from a recent theoretical approach of Rat et al. The latter consists in deriving transport properties in thermal plasmas from the solution of the Boltzmann's equation according to the Chapman-Enskog method keeping the coupling between electrons and heavy species.
Plasma composition is obtained from a non-equilibrium constant method and a stationary kinetic calculation. First, electrical and translational thermal conductivities are compared with those evaluated with the simplified theory of transport properties of Devoto and Bonnefoi. Non-negligible discrepancies occur reaching more than 30 and 40 % respectively for the electrical and electron thermal conductivities at $T_e = 15000$ K for $\theta = 2$. Second, the dependence with T_e of electrical and total thermal conductivities (including translational, internal and reactional contributions) and viscosity is examined as a function of the method of calculation of plasma composition and the non-equilibrium parameter $\theta = T_e/T_h$. It is emphasized that non-equilibrium transport coefficients are strongly dependent on the method of plasma composition.
Keywords: transport coefficients, argon-hydrogen, two-temperature, thermal plasma.

1. INTRODUCTION

With the development of plasma diagnostic techniques highlighting the non-equilibrium character of thermal plasmas, plasma processes modeling has to take into account different kinetic temperatures between electrons and heavy species. These models require the plasma composition and transport coefficients.
Recently, the simplified theory of transport properties [1,2], often used in two-temperature modeling (see for example [3,4]), has been questioned [5] when calculating combined diffusion coefficients [6] from the simplified expression of diffusion fluxes. Thus, an alternate approach has been proposed keeping a coupling between electrons and heavy species in the calculation of transport coefficients [7].
This paper is devoted to the calculation of two-temperature transport coefficients in an argon-hydrogen mixture at atmospheric pressure from the approach of Rat et al. [7]. The influence of the method of calculation of plasma composition on transport coefficients is also investigated. The second part of this paper deals with the two-temperature Ar-H_2 plasma composition, obtained from a stationary kinetic calculation and a two-temperature constant equilibrium method. The third section shows, first, a comparison between transport coefficients calculated from [2] and [7] theories, and second, the dependences of results of transport coefficients (electrical conductivity, viscosity and thermal conductivity) with the plasma composition and the ratio $\theta = T_e/T_h$, where T_e is the kinetic temperature of electrons and T_h that of heavy species.

2. COMPOSITION

The plasma composition, which is a prerequiste to obtain transport coefficients, is calculated assuming chemical equilibrium. An atmospheric Ar-H_2 plasma has been considered with nine species: e, Ar, Ar^+, Ar^{2+}, H_2, H, H_2^+, H^+ and ArH^+.

The plasma composition is obtained using a two-temperature (2T) constant equilibrium method (^{KpC}) and a stationary kinetic calculation (KinC). The description of these methods of calculation and the choice of species have been explained elsewhere [8,9].

Firstly, figure 1 shows the atmospheric plasma composition of the Ar-H_2 (50mol%) mixture at equilibrium as function of temperature.

It is observed that the dissociation of H_2 is maximum ($n_{H_2} = n_H$) at about 3800 K, the number density of hydrogen atoms increasing by nine orders of magnitude between 1000 and 3800 K. The ions ArH^+ and H_2^+ are not dominant. At about 15000 K, the electron number density reaches a plateau, as does the number density of H^+ and Ar^+ (at least up to 25000 K).

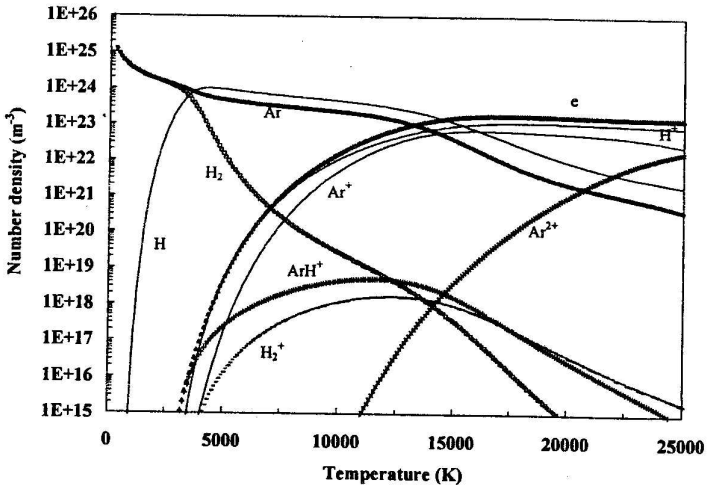

Figure 1 : Evolution of the equilibrium composition with temperature of an $Ar-H_2$ (50mol%) mixture at atmospheric pressure.

Secondly, a comparison between both methods of calculation of non-equilibrium plasma composition is presented below. Figures 2 and 3 depict respectively the evolution of the Ar-H_2 (50 mol %) plasma composition at atmospheric pressure for $\theta = 1.6$ respectively obtained from KinC and KpC calculations.

First, in figure 2, a strong discontinuity is observed at $T_e = 11000$ K, which is denoted in the following as T_D, the discontinuity temperature. This kind of discontinuity is typical of multi-temperature stationary kinetic calculations [10]. Dissociation follows the same evolution as at equilibrium, that is for $T_e < 5000$ K the electron number density n_e is negligible. This induces a shift of dissociation to the higher electron temperature when $\theta = T_e/T_h$ increases.

It has also to be noted that the heavy species temperature T_e/θ at which electrons, Ar^+, H^+, H_2^+ and ArH^+ appear at a number density of 10^{15} m^{-3} in figure 2, corresponds to that at equilibrium. This means that, below the discontinuity temperature T_D, ionization is controlled by charge transfer and dissociative recombination reactions, which prevent hydrogen and argon atoms from ionizing [9].

However, when the number density of hydrogen molecules is too small ($\approx 5.10^{20}\ m^{-3}$), charge transfer reactions become inefficient and do not limit anymore ionization of hydrogen and argon atoms, inducing an avalanche ionization and a discontinuity in plasma composition curves. It may be pointed out that an ionization delay is observed in figure 2 around $T_e = 5000$ K with respect to figure 3, due to the dissociative recombination reactions previously invoked. Finally, an atypical evolution of the number density of the Ar^+ ion occurs for electron temperatures above that of the discontinuity (fig 2).

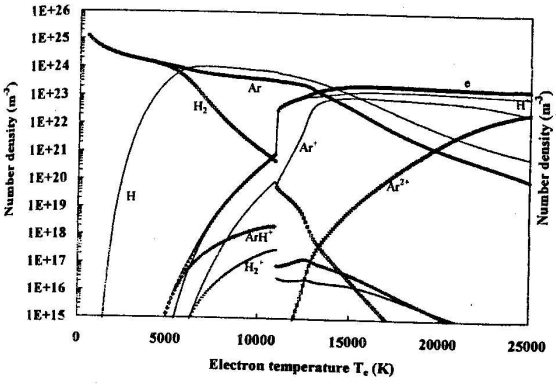

Figure 2: Evolution of the non-equilibrium composition with the electron temperature of an $Ar-H_2$ (50% mol) mixture at atmospheric pressure for θ=1.6 obtained using the stationary kinetic calculation

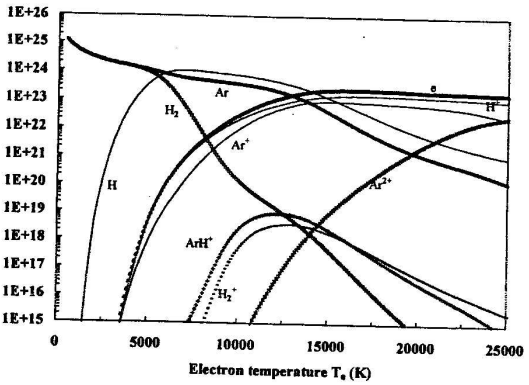

Figure 3: Evolution of the non-equilibrium composition with the electron temperature of an $Ar-H_2$ (50% mol) mixture at atmospheric pressure for θ=1.6 obtained by the two-temperature equilibrium constant method.

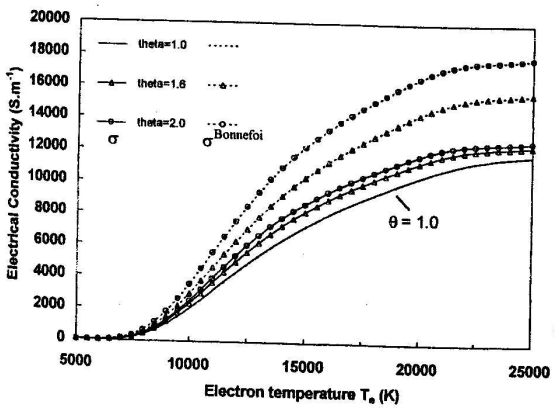

Figure 4: Evolution of the electrical conductivity with the electron temperature calculated from [7] and from the simplified theory of transport properties of Bonnefoi [2] in a Ar-H_2 (50mol%) plasma for different values of $\theta = T_e/T_h$ (composition by two-temperature equilibrium constant method).

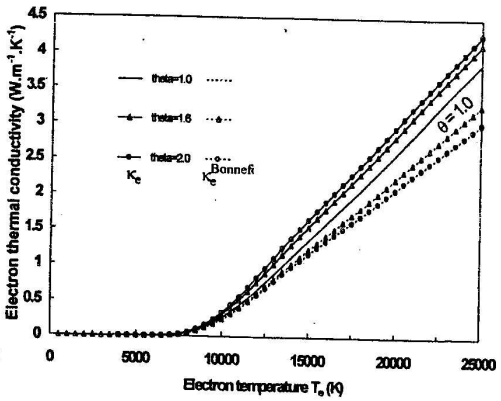

Figure 5: Evolution of the electron translational thermal conductivity with the electron temperature calculated from [7] and from the simplified theory of transport properties of Bonnefoi [2] in a Ar-H_2 (50mol%) plasma for different values of $\theta = T_e/T_h$ (composition by two-temperature equilibrium constant method).

3. TRANSPORT COEFFICIENTS

Transport coefficients are calculated at atmospheric pressure for temperatures up to 25000 K using the data basis of collision integrals established in [8].
The calculation of the electrical conductivity and viscosity are performed to the second approximation order and to the third order for the translational thermal conductivity.

3.1 Comparison with the simplified theory of transport properties [2]

In this section, electrical conductivity (figure 4) and translational electron thermal conductivity (figure 5) calculated from the approach of Bonnefoi [2] and that of Rat et al. [7] are compared for a non-equilibrium argon-hydrogen mixture at atmospheric pressure.
First, a good agreement is found at equilibrium. However, discrepancies are observed, between the two approaches, not only for the electrical conductivity but also for the translational electron thermal conductivity.

3.2 Electrical conductivity

The evolution, calculated with the approach of Rat [7], of the electrical conductivity σ of an $Ar-H_2$ (50mol%) mixture with the electron kinetic temperature is shown in figure 6 using a composition calculated by the stationary kinetic calculation (KinC) and the 2T equilibrium constant method (KpC) for θ=1.6 and θ=2.0.
It can be noted that the discontinuity found in composition curves obtained by KinC also occurs in the electrical conductivity at about 11000 K. For $T_e > T_D$, results obtained are almost independent of θ and the method of calculation of composition whereas, for $T_e < T_D$, KinC introduces an ionization delay due to the dissociative recombination reactions and consequently values of σ_{KinC} are much lower than those of σ_{KpC}.

3.3 Viscosity

The evolution with the electron temperature of the viscosity of an $Ar-H_2$ (50 mol %) mixture, using a composition calculated by the stationary kinetic calculation and the 2T equilibrium constant method, is depicted in figure 7 for $\theta = 1.6$ and $\theta = 2.0$.
A discontinuity, at around 11000 K, occurs in the KinC viscosity. The maximum of the latter is shifted to a higher electron temperature with respect to the KpC viscosity. This is due to the fact that an ionization delay occurs in the KinC viscosity, which consequently increases with temperature until the discontinuity is reached.

3.4 Thermal conductivity

Thermal conductivity is calculated with respect to the heavy species temperature gradient taking into account different contributions: translational and internal as well as reactional. The latter has been defined independently of the method of calculation of plasma composition [9].

In figure 8, the evolution with the electron temperature of the total thermal conductivity of an $Ar-H_2$ (50mol%) mixture is given using compositions calculated both by the KinC and KpC methods for $\theta = 1.6$ and $\theta = 2.0$.
For $\theta = 1.6$, a good agreement is observed between the dissociation peaks for both the KinC and KpC methods. However, for $\theta = 2.0$, the maximum value of the KpC dissociation peak is higher than that of the KinC.

Furthermore, for a temperature range of 8000-11000 K, the KinC method leads to an ionization delay of argon atoms, $\kappa_{tot}(\text{KinC}) < \kappa_{tot}(\text{KpC})$, but at temperatures above the avalanche phenomena, n_{Ar^+} increases faster, giving $\kappa_{tot}(\text{KinC}) > \kappa_{tot}(\text{KpC})$.

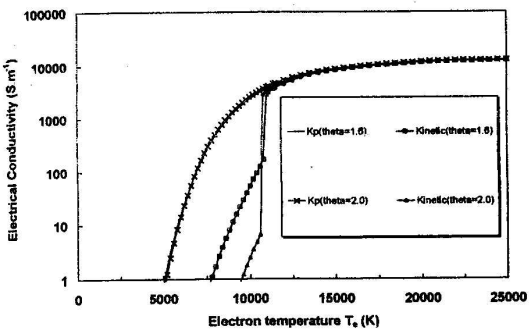

Figure 6: Evolution of the electrical conductivity σ with the electron kinetic temperature calculated from [7] at atmospheric pressure of an $Ar-H_2$ (50mol%) mixture using compositions calculated by the stationary kinetic calculation (Kinetic) and the two-temperature equilibrium constant method (Kp) for $\theta = 1.6$ and $\theta = 2.0$.

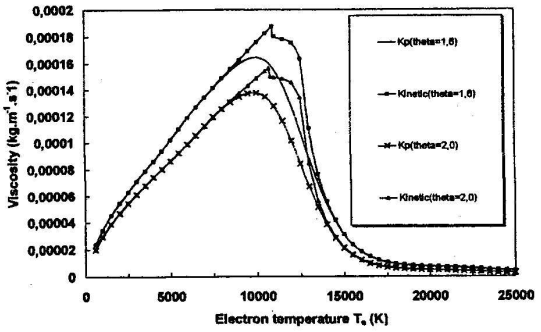

Figure 7: Evolution of viscosity with the electron temperature calculated from [7] at atmospheric pressure of an $Ar-H_2$ (50mol%) mixture using compositions calculated by the stationary kinetic calculation (Kinetic) and the two-temperature equilibrium constant method (Kp) for $\theta = 1.6$ and $\theta = 2.0$.

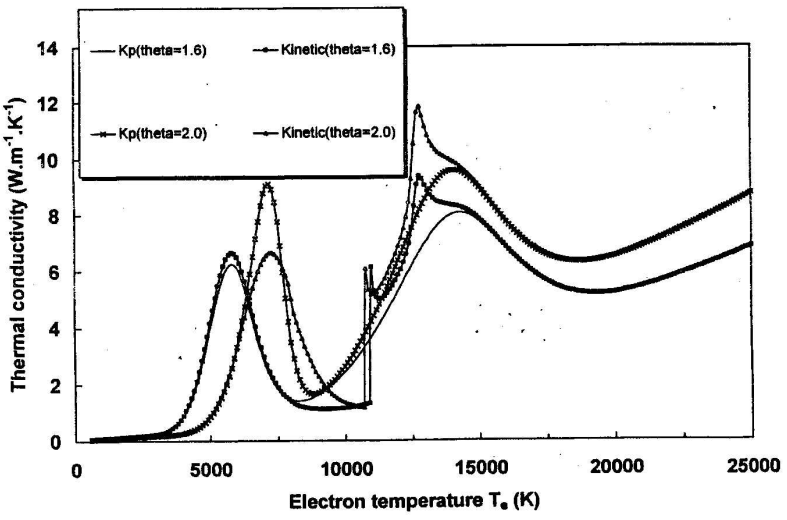

Figure 8: Evolution of the total thermal conductivity with the electron temperature calculated from [7] at atmospheric pressure of an $Ar-H_2$ (50mol%) mixture using compositions calculated by the stationary kinetic calculation (Kinetic) and the two-temperature equilibrium constant method (Kp) for $\theta = 1.6$ and $\theta = 2.0$.

4. CONCLUSION

This paper is devoted to the calculation of transport coefficients of a non-equilibrium argon-hydrogen plasma at atmospheric pressure from the theory of Rat et al taking into account the coupling between electrons and heavy species [7]. The kinetic temperature of electrons T_e is assumed to be different from that of heavy species T_h, and chemical equilibrium is supposed to be achieved.

First, a comparison between transport coefficients calculated from [7] and the simplified theory of transport properties [1,2] shows that the latter introduces large discrepancies for an argon-hydrogen plasma as also previously highlighted for a pure argon plasma [11].

Moreover, it has been shown that the method of calculation of plasma composition has a strong influence on transport coefficients. Particularly, a stationary kinetic calculation introduces a discontinuity in plasma composition curves, and consequently in transport coefficients curves. Finally, the value of the non-equilibrium parameter $\theta = T_e/T_h$ strongly influences transport coefficients (except the electrical conductivity for $T_e > 11000\,K$), even for low values of θ between 1 and 2.

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